

SCIDAC PROGRAM (Scalable Computational Tools for Discovery and Design: Excited State Phenomena in Energy Materials)

PUBLICATIONS – 1 OCT 2013 to 1 OCT 2014

Steve Louie – Lead PI

Primary Publications

1. "Improved quasiparticle wavefunctions and mean field for G_0W_0 calculations: Initialization with the COHSEX operator", M. Jain, [J. Deslippe](#), G. Samsonidze, [M. L. Cohen](#), J. R. Chelikowsky, and [S. G. Louie](#), *Phys. Rev. B* vol. 90, p. 115148, **2014**. DOI: 10.1103/PhysRevB.90.115148.
2. "Effects of self-consistency and plasmon-pole models on GW calculations for closed-shell molecules", J. Lischner, S. Sharifzadeh, [J. Deslippe](#), [J. B. Neaton](#), and [S. G. Louie](#), *Phys. Rev. B* vol. 90, p. 115130, **2014**. DOI: 10.1103/PhysRevB.90.115130.
3. "Ab Initio Study of Hot Carriers in the First Picosecond after Sunlight Absorption in Silicon", M. Bernardi, D. Vigil-Fowler, [J.B. Neaton](#), and [S.G. Louie](#), *Phys. Rev. Lett.*, vol. 112, p. 257402, **2014**. DOI: 10.1103/PhysRevLett.112.257402.
4. "Outer-valence electron spectra of prototypical aromatic heterocycles from an optimally-tuned range-separated hybrid functional", D. A. Egger, S. Weismann, S. Refaelly-Abramson, S. Sharifzadeh, M. Dauth, R. Baer, S. Kummel, [J. B. Neaton](#), E. Zojer, and L. Kronik, *J. Chem. Theory Comput.* vol. 10, p. 1934, **2014**. DOI: 10.1021/ct400956h.
5. "Effect of Spin Fluctuations on Quasiparticle Excitations: First-principles Theory and Application to Sodium and Lithium", J. Lischner, T. Bazhirov, A.H. MacDonald, [M.L. Cohen](#), and [S.G. Louie](#), *Phys. Rev. B* vol. 89, p. 081108, **2014**. DOI: 10.1103/PhysRevB.89.081108.
6. "First-principles DFT+GW Study of Oxygen Vacancies in Rutile TiO₂", A. Malashevich, M. Jain, and [S.G. Louie](#), *Phys. Rev. B* vol. 89, p. 075205, **2014**. DOI: 10.1103/PhysRevB.89.075205.

Secondary Publications

1. "Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor", M. M. Ugeda, A. J. Bradley, S.-F. Shi, F. H. da Jornada, Y. Zhang, D. Y. Qiu, W. Ruan, S.-K. Mo, [Z. Hussain](#), Z.-X. Shen, [F. Wang](#), [S. G. Louie](#), and [M. F. Crommie](#), *Nature Materials* Advance Online Publication, **2014**. DOI: 10.1038/nmat4061.
2. "Probing excitonic dark states in single-layer tungsten disulphide", Z. Ye, T. Cao, K. OBrien, H. Zhu, X. Yin, Y. Wang, [S. G. Louie](#), and [X. Zhang](#), *Nature* vol. 513, p. 214-218, **2014**. DOI: 10.1038/nature13734.
3. "Tuning Many-body Interactions in Graphene: The Effects of Doping on Excitons and Quasiparticle Lifetimes", K. F. Mak, F. H. da Jornada, K. He, [J. Deslippe](#), N. Petrone, J. Hone, J. Shan, [S. G. Louie](#), and T. F. Heinz, *Phys. Rev. Lett.* vol. 112, p. 207401, **2014**. DOI: 10.1103/PhysRevLett.112.207401.

4. "First-principles Study of Quasiparticle Energies of a Bipolar Molecule in a Scanning Tunneling Microscope Measurement", G. Samsonidze, [M.L. Cohen](#), and [S.G. Louie](#), *Comp. Mat. Sci.* vol. 91, p.187, **2014**. DOI: 10.1016/j.commatsci.2014.04.049.
5. "Satellite Structures in the Spectral Functions of the Two-dimensional Electron Gas in Semiconductor Quantum Wells: A *GW* Plus Cumulant Study", J. Lischner, D. Vigil-Fowler, and [S.G. Louie](#), *Phys. Rev. B* vol. 89, p. 125430, **2014**. DOI: 10.1103/PhysRevB.89.125430.